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Transmutation analysis of realistic low-activation steels for magnetic fusion reactors and IFMIF

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Abstract

A comprehensive transmutation study for steels considered in the selection of structural materials for magnetic and inertial fusion reactors has been performed in the IFMIF neutron irradiation scenario, as well as in the ITER and DEMO ones for comparison purposes. An element-by-element transmutation approach is used in the study, addressing the generation of: (1) H and He and (2) solid transmutants. The IEAF-2001 activation library and the activation code ACAB were applied to the IFMIF transmutation analysis, after proving the applicability of ACAB for transmutation calculations of this kind of intermediate energy systems.

Key words: Fusion Reactor Materials (F0800), Steels, Ferritic/Martensitic, Low Activation (S1000)

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1. Introduction

The reduced activation (RA) materials based on modified ferritic/martensitic steels (Fe-Cr-W-V-Ta), V-Cr-Ti alloys and SiC composites are in permanent progress by the international fusion materials community [1]. However, there is a global consensus that the qualification of materials in a suitable test environment is inevitable for design, construction and safe operation of DEMO fusion reactors. In this sense, an appropriated fusion materials irradiation facility has been proposed: the International Fusion Material Irradiation Facility (IFMIF). In exploring if fusion relevant irradiation damage conditions can be realised in IFMIF, evaluation of both displacement damage and solid/gaseous transmutants is necessary.

Our concern here is to perform a comprehensive transmutation study of some low activation steels for irradiation simulations in the High Flux Test Module (HFTM) of the IFMIF neutron source. Also, we intend to show that an updated version of the ACAB activation code is able to deal properly with this problem using the IEAF-2001 activation library. Calculations for the first wall of ITER and DEMO magnetic fusion reactor are also accomplished and results are compared with those of the IFMIF simulation facility.

In earlier work, different inventory computational codes, previously developed for fusion applications, have shown to be reliable for IFMIF applications with appropriated modifications [2, 3]. Following the same trend, this capability has been incorporated into the ACAB code [4]. Applications to transmutation of different steels and some particular elements have been performed [3]. Here, the analysis is extended to all the potential elements to be present in steels, and the study is carried out by means of an element-by-element evaluation. This approach allows us to apply the transmutation results for elements straightforward to study transmutation of any material consisting of some of the considered elements, as well as to analyse the different transmutation performance of the different materials.

In this transmutation study, we have selected some proposed candidate steels for first structural wall [5]: i) several existing 300 series stainless steels (SS304, ITER316 and primary candidate alloy PCA), and ii) some magnetic and inertial fusion energy aimed RA ferritic steels (F82H-IEA and EUROFER 97, and the ODS low activation ferritic steel LAF-3). The concentration of alloying and impurity elements can also be found in [5]. For the element-by-element study we have classified the constituents elements into three groups: i) Typical intended elements in RAFS as well as most of the intended ones in SS (B, C, N, O, Si, P, S, Ti, V, Cr, Mn, Fe, Y, Ta, W), ii) some of the impurity elements in RAFS as well as some of the intended elements in SS and Cr-Mo steels (Al, Co, Ni, Cu, Nb, Mo) and, iii) impurity elements common to all the steels (Zn, As, Se, Zr, Ru, Rh, Pd, Ag, Cd, Sn, Sb, Te, La, Ce, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Hf, Os, Ir, Pt, Au, Pb, Bi).

2. Computational methodology and validation process

In neutron fusion environments, transmutation calculations have been performed using the ACAB radionuclide generation/depletion code [4]. The nuclear data used are those from European Activation File EAF-2003 (EAF_XS and EAF_DECAY) [6].

In IFMIF, transmutation calculations have been conducted with an updated version of ACAB code that can handle the numerous reaction channels for neutron energies over 20 MeV. The updated ACAB code does not rely on a table of fixed reaction types, requiring only a list of resultant isotopes and cross-sections for the production of each. In IFMIF, the neutron source spectrum is extended up to ~55 MeV, with ~20% of the neutrons having energies above 15 MeV. The activation cross-section library processed for IFMIF is the Intermediate Energy Activation File IEAF-2001 [7]. This library contains the neutron activation cross-section files for 679 nuclides, including stable and isomeric states up to 150 MeV. We have used the group-wise IEAF-2001 library in GENDF format with 256 neutron energy structure. To be consistent with IEAF-2001, we have processed a complete decay library based on JEFF3.1 Decay Library (3,849 radionuclides) with an extra number of 135 radionuclides from other decay sources.

In order to validate our updated ACAB code for IFMIF calculations, we have tested our predictions with a set of integral activation experiments [8] having a neutron spectrum very close to IFMIF. In Table 1, we present the comparison of activation prediction for a sample of SS316. This steel has been irradiated during 7,525 s with a neutron flux of $4.10*10^{11}$ n/cm^2 s. We have adopted the average neutron flux in a 45-group energy structure at the centre position of the irradiated steel sample reported in Ref. [8]. The calculation-to-experiment ratios (C/E) obtained by ACAB/G-IEAF-2001 are shown in Table 1. For the most important radionuclides to the total activity and contact dose rate (^{56}Mn, ^{54}Mn, ^{57}Ni, ^{58}Co and ^{60}Co) the predictions have demonstrated a reasonable agreement, C/E ratios are between 0.7/1.3. For the rest of isotopes, larger deviations of C/E from unity were found, C/E ratios are between 0.02/4.45. These discrepancies can arise from: i) the activation cross section library, ii) the fact of neglecting the sequential charged-particle reactions, and iii) the uncertainties of the sample initial composition.

Our results are in general in good agreement with those obtained by ALARA and FISPACT codes [2, 3]. However, discrepancies up to 30% have been found for a few isotopes (^{52}Fe, ^{87m}Y). Both the different decay data libraries and the adopted neutron spectrum can explain these differences.

3. Transmutation element-by-element: Gaseous and solid transmutants

An extensive evaluation for three different neutron environments has been performed to assess the importance of the element-by-element transmutation in fusion materials. We have considered the IFMIF scenario (5.86 10^{14} n/cm^2 s, <E> ~6.95 MeV and wall loading 6.4 MW/m^2) in comparison with DEMO (13.0 10^{14} n/cm^2 s, <E> ~3.13 MeV and wall loading 3.5 MW/m^2) and ITER (3.90 10^{14} n/cm^2 s, <E> ~3.92 MeV and wall loading 1.2 MW/m^2). [2, 3]

Firstly, the H and He gas production is analyzed. H&He are generated by nuclear reactions (n,xH) or (n,xHe) on all nuclei. Their generation depends on both the neutron flux level and the neutron spectrum. In Table 2, we present the H&He production for from the initial the major-minor steel constituents and some impurities. For the most important ones, we have demonstrated that the generation of gaseous transmutants increases linearly as a function of irradiation time.

Secondly, the evolution of solid transmutants is investigated. In Table 3 we illustrate the most important element-by element transmutation processes in IFMIF under one year of irradiation time: the depletion of the initial Z element and the generation of new elements. Regarding major steel constituents, it is seen that the transmutation of W will increase the level of Ta and Os, approximately with the same ratio. The Cr will be transmuted mainly into V, and the Mn into Cr. The Ni will be transmuted into Co by (n,xH) reactions and into Fe by (n,xHe) reactions, 37% and 60%, respectively. And, Mo into Nb (52%), Zr and Ru. We have extended such element-by-element calculations to different irradiation times and we observed that the evolution for the most of the initial elements increase/decrease nonlinearly under irradiation time.

4. Transmutation in steels: Application to EUROFER

The element-by-element transmutation presented in Tables 2 and 3 leads to predict the transmutation performance of any material irradiated in IFMIF, DEMO and ITER. Figure 1 shows the total production of H&He for the selected steels under the different scenarios after one year of irradiation. These gaseous transmutant concentrations can be comparable to some initial steel constituents. The higher levels of H&He production are in PCA steel as a consequence of Ni concentration by (n,xH) and (n,xHe) reactions. Regarding IFMIF, the contribution for H generation is due to Cr(8.3%), Fe(47.5%) and Ni(41.5%). For He, the main generation is also due to Cr(9.2%), Fe(46.7%) and Ni(36.8%). For the rest of steels, iron produces the most important levels of H and He transmutants (~92% and ~84% respectively for EUROFER). Similar contributions are predicted in DEMO and ITER. The hard neutron spectrum in IFMIF and the high neutron level in DEMO lead to the higher H and He transmutation rates in comparison with ITER. We have also calculated the generation of H and He for DEMO and ITER with IEAF-2001 and EAF-2003 libraries. IEAF-2001 always over predicts the total generation of H and He, ~10% and ~3% respectively for EUROFER.

Table 4 shows the main transmutants of EUROFER in IFMIF, ITER and DEMO for different irradiation times. The most important transmutation effects are produced in IFMIF, the majority of steel constituents will not change under irradiation (Fe, Cr, C, ...) while some major and minor intended elements will do (B +7.3%, Ti +26%, V +10%, Mn +25%, Ta +2%, W -0.3%), new impurities generated are also important (Re 4.7 appm, Hf 1.3 appm, Be 2.3 appm, Mg 1.7 appm). In DEMO and ITER, we observed the significant generation of new elements such as Re and Os from W, and the depletion of B.

5. Conclusions

The updated version of ACAB code is able to deal with transmutation calculations in IFMIF facility using IEAF-2001 intermediate energy library. An integral experimental activation benchmark has been used to validate our system. The calculated results are in a quantitative agreement with the experimental data similar to that obtained with other computational approaches already validated for IFMIF applications.

The element-by-element analysis has been demonstrated as a helpful tool to easily analyse the transmutation performance of irradiated fusion materials. The contribution of each source-element to the generation of any transmutant product is obtained in a straightforward way.

IEAF-2001 over predicts the generation of gaseous transmutants, H and He, for ITER and DEMO compared to EAF-2003, and they have shown a linear behaviour with the irradiation time.

To complete this study, the impact of the activation cross section uncertainties on the IFMIF transmutation calculations will be estimated. The sensitivity/uncertainty Monte Carlo methodologies implemented in ACAB will make use of the recent EAF-2005 uncertainty library to perform this job. In addition, a more complete benchmarked of ACAB against the already validated computational methodologies used for activation and transmutation calculations of IFMIF will be performed.

Acknowledgments

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Table 1. Calculation-to-experiment ratios for the activity inventories induced in the SS-316 intermediate energy activation experiment [8].

Isotope	Decay time (h)	C/E	Isotope	Decay time (h)	C/E
Sc-46	49.68	2.03	**Ni-56**	49.68	1.60
Sc-48	49.68	1.56	**Ni-57**	49.68	1.30
V-48	49.68	2.64	**Y-87m**	49.68	0.40
Cr-48	49.68	4.45	**Y-87g**	49.68	0.48
Cr-49	1.66	0.82	**Y-88**	3600	1.00
Cr-51	49.68	1.02	**Zr-86**	49.68	0.03
Mn-52g	49.68	3.32	**Zr-88**	700	1.00
Mn-54	49.68	1.09	**Zr-97**	49.68	0.02
Mn-56	25.93	1.22	**Nb-90g**	49.68	0.45
Fe-52	25.93	1.22	**Nb-92m**	49.68	1.45
Fe-59	49.68	1.10	**Nb-95g**	49.68	1.58
Co-55	49.68	2.57	**Nb-95m**	49.68	1.18
Co-56	49.68	2.81	**Nb-96**	49.68	1.83
Co-57	49.68	1.03	**Mo-90**	49.68	1.48
Co-58g	49.68	1.19	**Mo-93m**	49.68	3.48
Co-60	49.68	1.21	**Mo-99**	49.68	1.26
Co-61	1.66	2.26	**Tc-99m**	49.68	1.26

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Table 2. H and He production (appm) from the major-minor steel constituents and some impurities under one year of irradiation time in the HFTM/IFMIF, DEMO and ITER. Calculations performed with ACAB/IEAF-2001.

		HFTM/IFMIF		DEMO		ITER	
	Element	**H**	**He**	**H**	**He**	**H**	**He**
Typical intended elements in RAFS as well as most of the intended ones in SS	**Cr**	1169	255	1312	230	552	97
	C	507	4289	2	7230	1	3105
	Mn	819	201	569	175	239	74
	P	2037	840	1828	1004	785	440
	S	5159	2418	5328	2344	2275	973
	V	699	285	744	106	324	44
	B	1085	1905	852	53057	343	13613
	N	1365	2221	1751	1605	660	655
	W	240	31	26	6	10	3
	Ta	241	18	33	3	13	1
	Si	2424	1395	2387	1627	1027	712
	Ti	865	316	849	224	360	94
	Fe	1551	301	1602	312	679	133
	Y	838	62	863	42	373	17
	O	794	1642	410	1435	174	640
Some of the impurity	**Cu**	1886	321	1947	314	851	134
	Ni	5699	999	6067	752	2477	322

elements in RAFS as well as some of the intended elements in SS and Cr-Mo steels	**Mo**	1089	190	1196	90	504	38
	Nb	674	117	364	74	153	31
	Al	1733	732	2602	927	1098	400
	Co	1297	273	2309	237	803	101
Impurity elements common to all the steels	**As**	721	168	473	90	203	37
	Sn	430	62	56	13	23	5
	Zr	650	64	476	57	200	24
	Sb	331	26	72	15	30	6
	Cd	375	54	146	21	61	9
	Bi	229	40	10	145	4	36
	Zn	2575	506	3097	564	1326	247
	Se	367	84	195	45	83	19
	Ag	776	127	463	60	195	25
	Tb	237	31	37	14	15	6
	Pb	199	44	7	4	3	2

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Table 3. Transmutants (appm) of the initial steel constituents under 1 year of irradiation time in HFTM/IFMIF. Calculations performed with ACAB/IEAF-2001.

	Initial	Transmutants (appm)				
Z	**Element**	**Z-2**	**Z-1**	**Z**	**Z+1**	**Z+2**
5	**B**	1326	458	-1885	0	0
6	**C**	482	347	-1695	0	0
7	**N**	1780	1422	-3372	0	0
8	**O**	1333	684	-2019	0	0
13	**Al**	262	1758	-2016	8	0
14	**Si**	1349	1095	-2425	0	0
15	**P**	202	1677	-1903	14	0
16	**S**	2490	2471	-4952	0	0
22	**Ti**	264	316	-556	0	0
23	**V**	4	694	-761	31	0
24	**Cr**	293	1995	-2331	0	0
25	**Mn**	81	1657	-1825	44	0
26	**Fe**	430	1153	-1669	0	0
27	**Co**	145	3255	-3425	5	0
28	**Ni**	3802	2339	-6238	1	0
29	**Cu**	255	4232	-4959	440	0
30	**Zn**	1341	2034	-3420	30	0
33	**As**	100	3299	-5101	1689	0
34	**Se**	112	289	-839	416	6
39	**Y**	35	3288	-3543	121	0
40	**Zr**	223	2027	-2409	23	129
41	**Nb**	83	2280	-2515	1	0

42	**Mo**	341	1009	-1912	516	18
44	**Ru**	431	484	-1964	955	72
45	**Rh**	200	3498	-5109	1312	0
46	**Pd**	150	834	-2227	1058	31
47	**Ag**	52	3776	-8938	2219	0
48	**Cd**	106	351	-1251	665	63
50	**Sn**	102	95	-651	410	2
51	**Sb**	1	4437	-7481	3019	0
52	**Te**	47	160	-3454	3215	28
57	**La**	40	578	-969	84	0
58	**Ce**	97	3215	-4048	705	21
62	**Sm**	137	309	-2372	1867	13
63	**Eu**	17	1782	-3735	1922	0
64	**Gd**	20	306	-2089	1496	206
65	**Tb**	17	1013	-2454	1438	0
66	**Dy**	25	433	-836	340	1
67	**Ho**	4	3672	-8545	4823	0
68	**Er**	81	3092	-4555	1210	9
69	**Tm**	94	7420	-8388	859	0
70	**Yb**	57	646	-2299	1273	31
71	**Lu**	14	2080	-2934	841	0
72	**Hf**	33	712	-1630	123	0
73	**Ta**	4	4451	-5709	1890	0
74	**W**	108	1611	-3205	1430	1
76	**Os**	48	206	-3285	2674	5
77	**Ir**	6	3593	-9065	3738	0
78	**Pt**	161	339	-1296	566	8
79	**Au**	27	9138	-10663	1459	0
82	**Pb**	41	442	-585	8	0
83	**Bi**	15	953	-1006	15	0

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Table 4. Transmutation (appm) of EUROFER constituents under different irradiation times -1, 3 and 5 full power years (fpy)- in the HFTM/IFMIF and one year in DEMO and ITER. Calculations performed with ACAB/IEAF-2001.

EUROFER Initial composition		**IFMIF (appm)**			**DEMO (appm)**	**ITER (appm)**
Element	**(appm)**	**1 fpy**	**3 fpy**	**5 fpy**	**1 fpy**	**1 fpy**
H	**--**	1500	4493	7477	1556	659
He	**--**	319	961	1609	342	147
Li	**--**	0.3	0.9	1.5	2.9	0. 8
Be	**--**	2.3	7.1	11.8	3.0	1.3
B	**51**	3.7	11.1	18.4	-1.5	-0.2
C	**4860**	-6.1	-18.3	-30.4	-9.5	-4.3
N	**1191**	-3.8	-11.3	-18.8	-3.7	-1.4
O	**347**	-0.70	-2.11	-3.50	-0.53	-0.24
Mg	**--**	1.7	5.1	8.4	2.2	0.9
Al	**206**	0.69	2.04	3.37	-0.003	-0.01
Si	**990**	-2.0	-6.2	-10.3	-1.9	-0.8
P	**90**	0.04	0.10	0.16	0.14	0.05
S	**87**	-0.43	-1.26	-2.08	-0.48	-0.20
Ti	**116**	30	103	183	29	12
V	**2183**	221	687	1149	235	94
Cr	**96236**	164	737	1420	73	35

Mn	**4048**	1014	3582	6738	921	385
Fe	**885880**	-1478	-5174	-9526	-1282	-568
Co	**47**	0.03	-0.10	-0.28	2.28	0.51
Ni	**47**	-0.11	-0.33	-0.53	0.20	0.03
Cu	**44**	-0.22	-0.65	-1.07	-0.49	-0.16
Nb	**6**	0.01	0.04	0.06	0.01	0.005
Mo	**29**	-0.06	-0.16	-0.27	-0.13	-0.04
Hf	**--**	1.3	4.8	9.0	1.3	0.6
Ta	**215**	4	17	30	-17	-3
W	**3327**	-10	-39	-68	-129	-33
Re	**--**	5	17	29	132	34
Os	**--**	0.005	0.060	0.165	13.7	0.8

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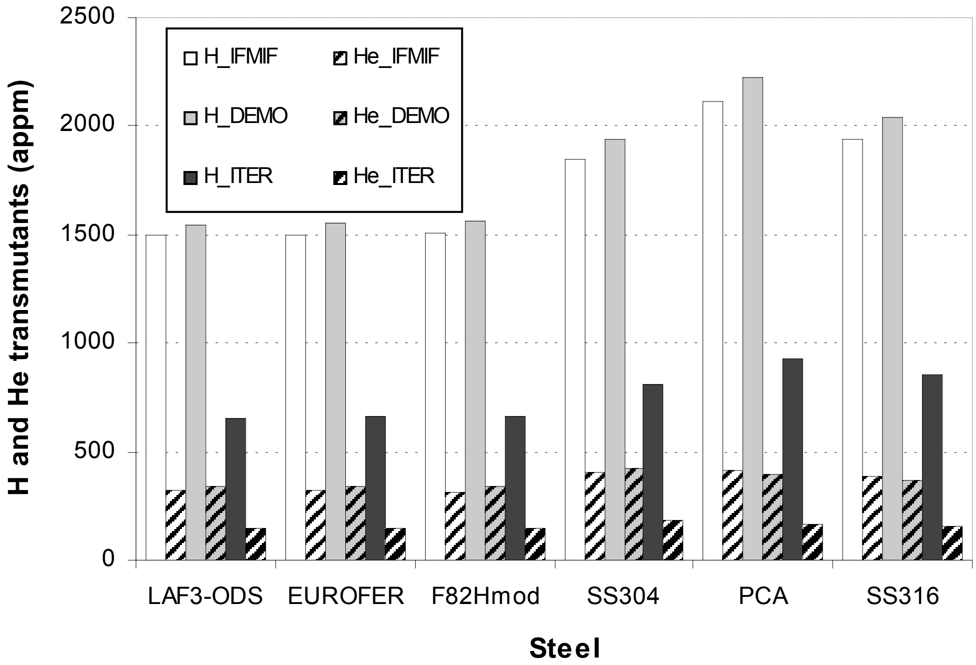

Figure 1. H and He (appm) production under one year of irradiation time in HFTM/IFMIF, DEMO and ITER for different steels. Calculations performed with ACAB/IEAF-2001.